A Material Model for High-strain-rate Applications, Including Phase Transformations, Material Anisotropy, and Damage

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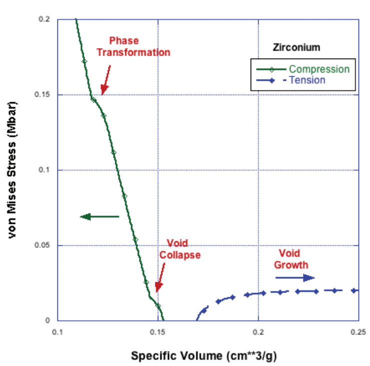
A thermodynamic framework has been used to develop a macro-mechanical model for high-strain-rate deformations. The model includes the effect of nonlinear elasticity (an equation of state), solid-solid phase transformations, plasticity, and damage. Phase transformations are addressed using either a free-energy or an equilibrium-phase diagram. An anisotropic inelastic potential is used to model the combined effects of plasticity and ductile damage. The model is being implemented into an engineering design computational framework and validated using small-scale experimental data.

There are numerous applications, which involve high-strain rates and high pressures. Impact, penetration, and weapons performance scenarios are examples of representative applications. The physical processes, which are encountered during high-rate deformations, may include nonlinear elasticity, plasticity, phase transformations, and damage. Nonlinear elasticity or equations of state are necessary to accurately model the material response to shock loading conditions. Coupled effects, including the ability of plasticity to inhibit a material from transforming back to a parent phase, for example, also represent important effects, which must be modeled. As larger stress states are encountered, damage nucleation, growth, and coalescence must be considered. These phenomena have their basis in the evolution of the material microstructure. However, macro-mechanical models are still necessary to address engineering applications.

Fig. 1. Pressure versus specific volume for uniaxial compression and tension of zirconium.



A macro-mechanical model has been developed that is based on thermodynamic considerations. To address phase transformations, the approach may utilize free energies for each phase or an equilibrium-phase diagram, depending on the availability of data. An anisotropic yield surface for the combined phenomena of plasticity and damage is considered to address the effects of material texture, rate dependence, and ductile failure. The thermodynamic framework, in general, relies on both elastic (free energy) and inelastic potentials. The total specific Helmholtz free energy for a mixture of phases is provided as the mass fraction average of the free energies of each of the k-constituents [$\psi^k(\bar{\bar{\varepsilon}}^e, T, D, \varepsilon^p)$] and a component due to mixing (ψ^{mix}):

$$\psi(\bar{\bar{\varepsilon}}^e, T, D, \varepsilon^p, \bar{\bar{\varepsilon}}^i, m) = \sum_k m_k \psi_k(\bar{\bar{\varepsilon}}^e, T, D) + \psi^{mix}(\bar{\bar{\varepsilon}}^i, m) \quad (1)$$

In equation (1), m_k is the mass fraction of each constituent, ψ_k is the free energy of the kth constituent, $\bar{\bar{\varepsilon}}^e$ is the elastic strain, T is the temperature, D is a measure of material damage, and $\bar{\bar{\varepsilon}}^e$ is the inelastic strain. Also, ψ^{mix} is the free energy, which is a consequence of mixing of the phases. Example free energies may be found in the literature [1-3]. Substitution of the mixture free-energy [equation (1)] into the Clausius-Duhem inequality for the dissipation rate results in expressions for the generalized thermodynamics forces including the stress, entropy, plasticity (hardening), damage, transformation strain, and transformation kinetics [3].

Two inelastic potentials, related to the combined effects of plasticity and damage [$\phi^p(\bar{\bar{\Sigma}}, \varpi^p, \varpi^d)$] and phase transformations [$\phi^t(\Pi) = 0$], are postulated. The appropriate inelastic parameters then may be defined in terms of these potentials [3]:

$$d\bar{\bar{\varepsilon}}^p = \frac{\partial \phi^p}{\partial \bar{\bar{\Sigma}}} d\lambda^p, \qquad d\varepsilon^p = \frac{\partial \phi^p}{\partial \varpi^p} d\lambda^p$$

$$dD = \frac{\partial \phi^p}{\partial \varpi^d} d\lambda^p, \qquad dm = \frac{\partial \phi^t}{\partial \Pi} d\lambda^t \quad (2)$$

In equation (2), the thermodynamics variables are $\bar{\bar{\Sigma}} \equiv \bar{\bar{\sigma}} - \bar{\bar{\mu}}^i$ and $\Pi \equiv \bar{\bar{\Sigma}} : \bar{\bar{\Lambda}} - \mu^m$. The parameters $d\lambda^p$ and $d\lambda^t$ are the Lagrange multipliers for plasticity and phase transformations, which may be obtained from the consistency conditions ($d\phi^p = 0$ and $d\phi^t = 0$). Extensions of the Gurson surface [4] have been considered for an ellipsoidal void embedded within a perfectly plastic, anisotropic matrix [5]. In the current model development, it is assumed that the voids remain spheroidal. The flow surface can be written with respect to a Cartesian coordinate system [5]

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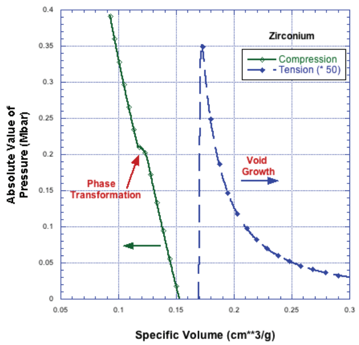

Fig. 2. Von Mises stress versus specific volume for uniaxial compression and tension of zirconium.

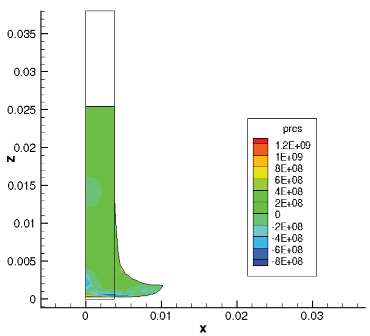

Fig. 3. A representative simulation of a Taylor impact experiment showing contours of pressure at t= 60 ms. The wire outline provides the original shape of the projectile.

associated with the axis of orthotropy for the matrix material:

$$\phi^p(P,\bar{\bar{s}},\phi) = \tfrac{3}{2}\bar{\bar{\sigma}} : \bar{\bar{\bar{\bar{M}}}} : \bar{\bar{\sigma}} - Y_s^2\left[1+(q_1\phi)^2 - 2q_1\phi\cosh\left(\frac{q_2\kappa P}{Y_0}\right)\right] = 0 \qquad (3)$$

In equation (3), $\bar{\bar{\bar{\bar{M}}}}$ is the anisotropy tensor for the matrix material, ϕ is the porosity, $\bar{\bar{\sigma}}$ is the Cauchy stress, P is the pressure, and κ is a material constant that is dependent on the material anisotropy. Strain rate dependent models may be used for the yield function (Y_s) of the solid or matrix material. The effective plastic strain of the matrix (solid) constituent (ε_s^p) is used as the hardening parameter in the model for the yield function. The matrix plastic strain is obtained from the equality between the plastic work of the composite and matrix materials [6]. The inelastic potential for the phase transformations is written in terms of the differences [2] of the free energies ($\dot{m}_k = f_k(\Delta g_{sk})$, where $g_{sk} = \psi_{sk} - v_{sk}\bar{\bar{\sigma}}_{sk} : \bar{\bar{\varepsilon}}_{sk}^e$ is the Gibb's free energy of each phase). If free energies are not available, then the kinetics may be obtained from an equilibrium phase diagram [7].

Finally, the total strain rate is decomposed into the elastic ($\dot{e}^e$), plastic ($\dot{e}^p$), and transformation ($\dot{e}^t$) rates. The plastic strain rate is obtained directly from the plastic potential [equation (2)]. Functional forms for the transformation strain rate may be found in the literature [3]. The evolution of porosity, in general, is composed of contributions due to void nucleation, growth, and coalescence. Classical approaches model the porosity growth [4,6] component as directly related to the change in the volumetric plastic strain [$d\varepsilon^p = tr(d\bar{\bar{\varepsilon}}^p)$] of the composite material $d\varphi = (1-\phi)\,d\varepsilon^p$.

A novel numerical technique [8] has been used to solve the resulting equations for the shear stress ($\tau = 3\bar{\bar{s}} : \bar{\bar{s}}/2$), pressure ($P$), porosity ($\phi$), and plastic strain, once the kinetics of the transformation process have been addressed. An overstress approach is being considered to address the issues related to localization and the ensuing ill-possedness problems.

Single-cell simulations (Figs. 1 and 2) using the model demonstrate the ability of the model to capture porosity crush-up and phase transformations for a uniaxial compressive condition as well as the growth of damage for a uniaxial tensile condition. The model is being implemented into a finite-difference computational analysis. Experimental data will be used to validate the model. For example, plate impact and Taylor impact (Fig. 3) simulations will be used in comparisons with experimental data to explore the ability of the model to accurately capture material anisotropy, rate dependence, phase transformations, and damage.

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